

# Delocalized Qubits as a Computational Basis in the System of Interacting Spins

Alexander R. Kessel and Vladimir L. Ermakov \*

*Kazan Physico-Technical Institute,  
Kazan Science Center,  
Russian Academy of Sciences,  
Kazan 420029 Russia*

February 1, 2008

## Abstract

It is suggested to map the qubits into solid state NMR spin system collective states instead of the states of the individual spin. Such an approach introduces the stable computational basis without any additional actions and allows to obtain the universal set of quantum gates, which operation time is determined only by a RF pulse duration.

PACS No.: 03.65.-w, 03.67.-a, 76.60.-k.

## 1 Introduction

Nuclear magnetic resonance (NMR) provides an excellent proving ground for testing different quantum information processing (QIP) ideas. Due to combination of its good developed theory and sophisticated experimental technique the realization of the simplest quantum algorithms using standard NMR spectrometers turned out to be possible. At present time the achievements of liquid state (LS) NMR QIP are far beyond the capabilities of any other experimental methods.

This success of LS NMR QIP is due also to the fact that a clear correspondence was found between the abstract notion of a quantum mechanical bit - qubit and real physical object - nuclear spin. Namely, two qubit states  $|0\rangle$  and  $|1\rangle$  are mapped onto two possible spin  $1/2$  projections. As a computational basis the eigenfunctions  $|m\rangle$  of the Z-components of a nuclear spin are used, which commutates with the full Hamiltonian. For example, for two spin system this computational basis is written as follows:

---

\*e-mail: [ermakov@dionis.kfti.knc.ru](mailto:ermakov@dionis.kfti.knc.ru)

$$\begin{aligned} |00\rangle &= |m_1 = -1/2, m_2 = -1/2\rangle, & |01\rangle &= |m_1 = -1/2, m_2 = +1/2\rangle, \\ |10\rangle &= |m_1 = +1/2, m_2 = -1/2\rangle, & |11\rangle &= |m_1 = +1/2, m_2 = +1/2\rangle. \end{aligned} \quad (1)$$

where  $|m_1\rangle$  and  $|m_2\rangle$  are the nuclear spin Z-components eigenfunctions.

However, already now one can see the LS NMR QIP limitations and the next step is going to be the solid state (SS) NMR QIP [1]-[3]. The SS NMR essential feature is the existence of the spin-spin (exchange and dipole-dipole) interaction terms in the total Hamiltonian, which are not averaged to zero by thermal motions, and which contain not only Z, but also X and Y spin components. Due to this fact a single spin orientation becomes bad integral of motion. This means that such system stationary states do not correspond to definite values of the spins Z-component and the functions (1) become time dependent. To use these functions as a stable computational basis it is necessary to remove spin-spin interactions using special means [3]. For example a WAHUA multipulse sequence, consisting of four pulses, can be used for this purpose [4].

In this paper it is shown how in the system of interacting spins with spin Z-components not commuting with total Hamiltonian, one can introduce a stable computational basis, which does not require the continuous application of a multipulse sequences. The trick is that instead of the correspondence “one qubit” - “a pair of single spin states” one makes the correspondence “one qubit” - “a pair of collective spin states”. Using the virtual spin formalism language [5] it can be written as “one qubit” - “one virtual spin”, instead of “one qubit” - “one real spin”. Such approach is being developed in the framework of our program “Quantum computer: many levels instead of many particles” [6]. Unlike the previous cases, in which the virtual spins have been defined on the levels of the individual multilevel particle - on the spins 3/2 or 7/2 levels [6]-[7], in the present case they are defined on the collective levels of the interacting spins system. It means that a qubit is “delocalized” and there is no direct correspondence “one qubit” - “one particle”.

## 2 A simple model of two spins interaction

A universal quantum gate set consists of single qubit rotations and two-qubit CNOT gate [8]. In order to implement such a set it will be enough to use a simple two spin interaction model. Let it will be the system of two non equivalent nuclear spins  $I = 1/2$  and  $S = 1/2$ , connected by isotropic exchange interaction.

This system Hamiltonian is

$$\begin{aligned} \mathcal{H} &= \hbar\omega_0(I_z + S_z) + \hbar\delta/2(I_z - S_z) + \hbar J(\mathbf{I} \cdot \mathbf{S}), \\ \omega_0 &= (1/2)(\gamma_I + \gamma_S)H_0, \delta = -(\gamma_I - \gamma_S)H_0 \end{aligned} \quad (2)$$

where  $\gamma_I$  and  $\gamma_S$  - the nuclei giromagnetic ratios,  $J$  - the exchange integral,  $H_0$  - the external constant magnetic field.

This Hamiltonian eigenfunctions and corresponding eigenvalues are

$$\begin{aligned} |\psi_1\rangle &= |++\rangle \equiv |m_I = +1/2, m_S = +1/2\rangle, & E_1 &\equiv \hbar\varepsilon_1 = \hbar\omega_0 + (1/4)\hbar J \\ |\psi_2\rangle &= p|+-\rangle + q|-+\rangle, & E_2 &\equiv \hbar\varepsilon_2 = -(1/4)\hbar J + (1/2)\hbar\theta \\ |\psi_3\rangle &= p|-+\rangle - q|+-\rangle, & E_3 &\equiv \hbar\varepsilon_3 = -(1/4)\hbar J - (1/2)\hbar\theta \\ |\psi_4\rangle &= |--\rangle, & E_4 &\equiv \hbar\varepsilon_4 = -\hbar\omega_0 + (1/4)\hbar J \end{aligned} \quad (3)$$

where  $p = \cos(\phi/2)$ ,  $q = \sin(\phi/2)$ ,  $\theta^2 = J^2 + \delta^2$ ,  $J/\delta = \tan(\phi)$ ,  $-\pi/2 \leq \phi \leq \pi/2$ .

This system has four allowed transitions with the following frequencies and relative intensities:

$$\begin{aligned} \varepsilon_{12} &= \omega_0 + (1/2)J - (1/2)\theta, & P_{12} &\propto |\langle\psi_1| I_x + S_x |\psi_2\rangle|^2 = 1 + \sin(\phi), \\ \varepsilon_{13} &= \omega_0 + (1/2)J + (1/2)\theta, & P_{13} &\propto |\langle\psi_1| I_x + S_x |\psi_3\rangle|^2 = 1 - \sin(\phi), \\ \varepsilon_{24} &= \omega_0 - (1/2)J + (1/2)\theta, & P_{24} &\propto |\langle\psi_2| I_x + S_x |\psi_4\rangle|^2 = 1 + \sin(\phi), \\ \varepsilon_{34} &= \omega_0 - (1/2)J - (1/2)\theta, & P_{34} &\propto |\langle\psi_3| I_x + S_x |\psi_4\rangle|^2 = 1 - \sin(\phi), \end{aligned} \quad (4)$$

Fig. 1 depicts the energy levels of this system. This simple system allows exact solution and manifests the specific features and advantages of the proposed information coding – the so-called “virtual spin formalism”. In a case of the more general interaction (anisotropic exchange or dipole-dipole one) all necessary expressions can be obtained using perturbation theory.

### 3 Computational basis in the virtual spin representation

The four dimensional Hilbert space, spanned on eigenfunctions (3), can be considered as a direct product of the pair of virtual spins  $R = 1/2$  and  $S = 1/2$  two-dimensional Hilbert spaces [6]. It means that the eigenfunctions (3) of Hamiltonian (2) can be taken to form the computational basis for the two qubit system, thus:

$$\begin{aligned} |00\rangle &= |\psi_1\rangle, & |01\rangle &= |\psi_2\rangle, \\ |10\rangle &= |\psi_3\rangle, & |11\rangle &= |\psi_4\rangle. \end{aligned} \quad (5)$$

This notation means that the qubit corresponds to the virtual spin, so:

$$\begin{aligned} |0_Q\rangle &= |m_Q = -1/2\rangle, & |1_Q\rangle &= |m_Q = +1/2\rangle, \\ |0_R\rangle &= |m_R = -1/2\rangle, & |1_R\rangle &= |m_R = +1/2\rangle. \end{aligned} \quad (6)$$

and two qubit states correspond to the computational basis:

$$\begin{aligned} |00\rangle &= |m_Q = -1/2, m_R = -1/2\rangle, & |01\rangle &= |m_Q = -1/2, m_R = +1/2\rangle, \\ |10\rangle &= |m_Q = +1/2, m_R = -1/2\rangle, & |11\rangle &= |m_Q = +1/2, m_R = +1/2\rangle. \end{aligned} \quad (7)$$

Now a resonance transition between any two real states of physical system admits the interpretation as virtual spin reorientations. For example, the irradiation of the transition  $\langle\psi_1|\leftrightarrow|\psi_2\rangle$  can be interpreted in the virtual spin representation as the Q spin rotation etc. Using the previous results [5]-[6] it can be shown, that in this two qubit system the universal gates set can be realized by means of the following resonance electromagnetic field pulses.

Logic operation:	Realization by transition(s):
Virtual spin Q rotation	$\langle\psi_1 \leftrightarrow \psi_2\rangle$ and $\langle\psi_3 \leftrightarrow \psi_4\rangle$
Virtual spin R rotation	$\langle\psi_1 \leftrightarrow \psi_3\rangle$ and $\langle\psi_2 \leftrightarrow \psi_4\rangle$
Controlled Q spin inversion $CNOT_{R\rightarrow Q}$	$\pi$ - pulse applied to $\langle\psi_3 \leftrightarrow \psi_4\rangle$
Controlled R spin inversion $CNOT_{Q\rightarrow R}$	$\pi$ - pulse applied to $\langle\psi_2 \leftrightarrow \psi_4\rangle$

where  $CNOT_{R\rightarrow Q}$  means that qubit Q undergoes the *NOT* operation, which is controlled by the state of qubit R, and  $\pi$  - pulse means the virtual spin Q rotation through the angle  $\pi$ . The corresponding resonance pulses are depicted on Fig. 2. It can be seen that all quantum gates can be implemented using just one pulse: for virtual spin rotation a double frequency pulse is necessary, whereas for *CNOT* operation - a single frequency pulse.

## 4 Conclusions

It was shown that the information coding onto virtual spins allows to implement a universal gate set in a solid state two interacting spin system. The advantages of this coding are connected with the fact, that spin-spin interactions can be large and that there is no need to use continuous irradiation with a multipulse sequence to have a stable computational basis. Large spin-spin interaction produces big resonance frequencies differences, which facilitate the selective resonance excitation of the individual transitions, desired for gates implementation. In addition, the gate operation time is under full control of an experimentalist and can be done short, whereas the coding using real spins requires time, defined by exchange interaction value (which is a given molecule property) and can be rather long.

It should be noted that the suggested approach can be useful also for LS NMR QIP in a case, when an exchange interaction is not averaged to spin Z-components. It can be used also for information coding onto any cluster of interacting particles of arbitrary nature. The only requirements are the existence of the proper selection rules for resonance transitions among cluster stationary states, on which a two virtual qubit system is defined. An example of the virtual qubit formalism applied to optical states of a single atom is given in the paper [9].

## References

- [1] J.A. Jones, “*NMR quantum computation: A critical evaluation*”, (quant-ph/0002085).
- [2] D.P. DiVincenzo, “*The physical implementation of quantum computation*”, (quant-ph/0002077).
- [3] D.G. Cory, R. Laflamme, E. Knill, L. Viola, T.F. Havel, N. Boulant, G. Boutis, E. Fortunato, S. Lloyd, R. Martinez, C. Negrevergne, M. Pravia, Y. Sharf, G. Teklemariam, Y.S. Weinstein, W.H. Zurek “*NMR Based Quantum Information Processing: Achievements and Prospects*”, (quant-ph/0004104).
- [4] J.S. Waugh, L.M. Huber, U.Haeberlen “*Approach to high resolution NMR in solids*”, Phys. Rev. Lett., 20:180–182, 1968.
- [5] A. R. Kessel, V. L. Ermakov, “*Multiqubit Spin*”, JETP Letters, Vol. **70**, pp. 61-65 (1999), (translation from Russian: Pis'ma v Zh. Eksp. Teor. Fiz. Vol. **70**, No. 1, pp. 59-63, 10 July 1999), (quant-ph/9912047).
- [6] A. R. Kessel, V. L. Ermakov, “*Virtual qubits - many levels instead of many particles*”, Zh. Eksp. Teor. Fiz. 117 (3), 517-525 (2000).
- [7] A. R. Kessel, V. L. Ermakov, “*Physical Implementation of Three-Qubit Gates on a Separate Quantum Particle*”, JETP Letters, Vol. 71(7), pp. 307-309 (April 10, 2000), (quant-ph/0002016).
- [8] Adriano Barenco, Charles H. Bennett, Richard Cleve, David P. DiVincenzo, Norman Margolus, Peter Shor, Tycho Sleator, John Smolin, Harald Weinfurter, “*Elementary gates for quantum computation*”, Phys. Rev. **A52**, 3457 (1995), (quant-ph/9503016).
- [9] V.L. Ermakov, A.R. Kessel, V.V. Samartsev, “*Four atomic optical energy levels as a two-qubit quantum computer register*”, SPIE Proceedings Vol. 4061, Paper 4061-11, pp.79-84, (quant-ph/0001090).

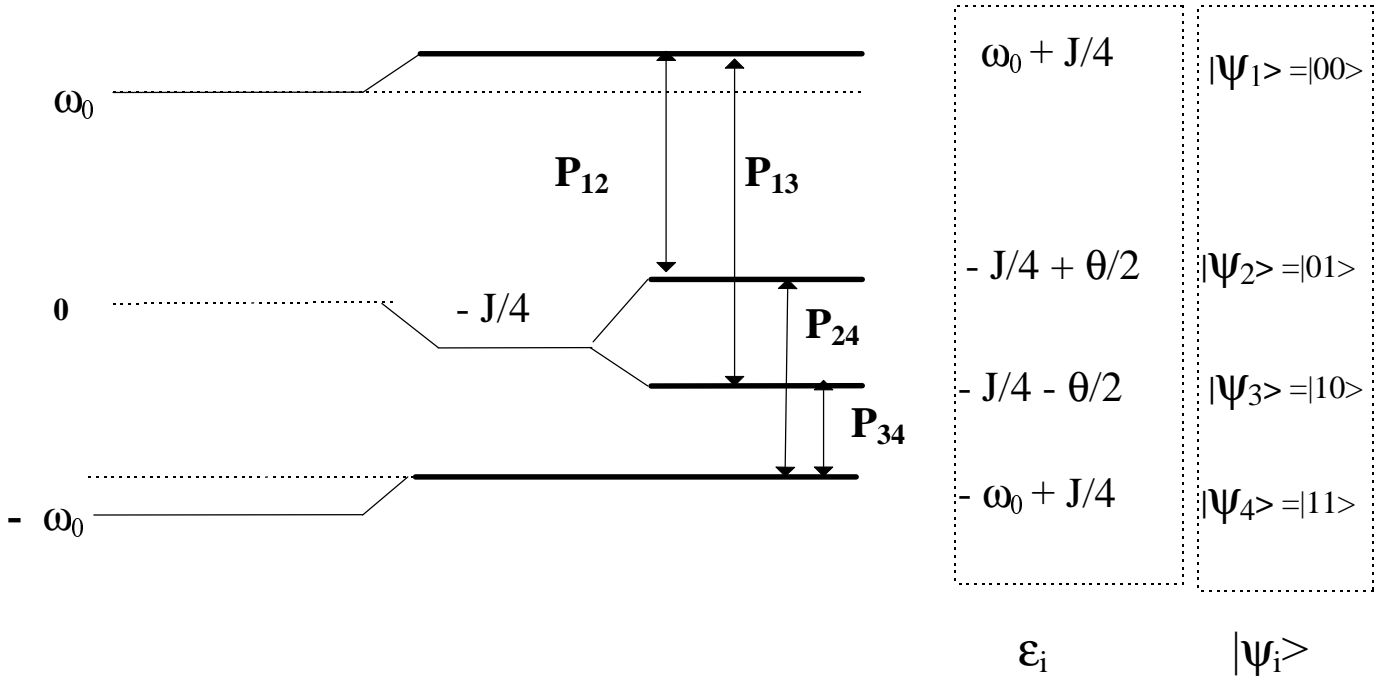


Fig.1. The energy levels, wave functions and the probabilities of the allowed transitions of the two non equivalent spins 1/2, connected by isotropic exchange interaction.

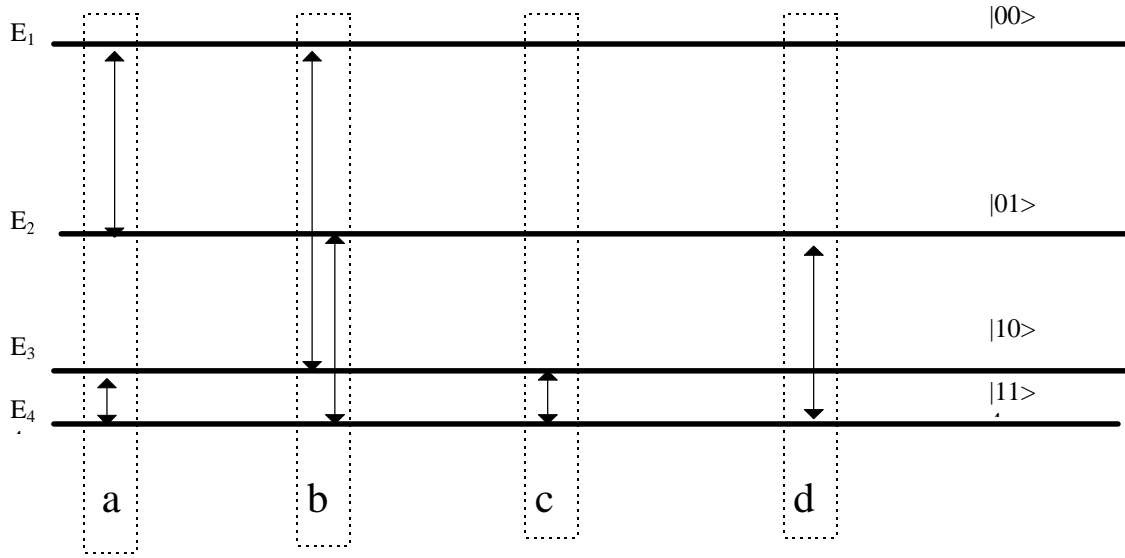


Fig. 2. The pulses which realize quantum logic gates when the qubits are encoded using virtual spin formalism. A dash box denotes a pulse (single or double frequency), whereas arrows means resonance transitions. a) virtual spin Q rotation; b) virtual spin R rotation; c)  $\text{CNOT}_{R \rightarrow Q}$ ; d)  $\text{CNOT}_{Q \rightarrow R}$ .